Steady-state currents in sharp stochastic ratchets

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We develop and analyze a model for particle transport in a stochastic ratchet with a periodic piecewise linear potential, with diffusion coefficient D, where the force is discontinuous in position and fluctuating in time via additive telegraph noise with correlation time τ . We find asymptotic formulas for the steady-state particle current J for large and small D and τ . For example, for small τ , the sharp corners in the potential lead to $J = O(\tau^2 \exp[-(D\tau)^{-1/2}]) + O(\tau^{5/2})$, in contrast to $O(\tau^3)$ when the potential is smooth. We show that diffusion can increase or decrease J, and derive an approximate equation for the value of D that maximizes J. [S1063-651X(99)05810-9]

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I. INTRODUCTION

In recent years there has been a surge of interest in noise-driven ratchets: stochastic dynamical systems with asymmetric periodic potentials, driven by a time-dependent external force [1]. There has been speculation that biological systems take advantage of the interplay between thermal diffusion and the fluctuating external force to transport molecules or vesicles [2-5]. Attempts have been made to use the principles of stochastic ratchets to design devices for separation of molecular or particulate moieties [6-10]. In the study of noise-induced transport, an important goal is to calculate the steady-state current of the system. If this is nonzero, it indicates that useful work is being extracted from the external force.

At the present stage of research, it is necessary to write down relatively simple dynamical systems to model the very complex biological or technological mechanisms. These models are studied in order to provide insight as to the interplay between the parameters that affect the current: the diffusion coefficient, and the spatial and temporal structures of the external forcing. From the solutions to such models, we wish to learn how actual systems may work and might be controlled [6,7,9]. For these purposes, we seek analytical insight deeper than can be provided by numerical solutions [11–13]. Such insight is necessary because even simple model ratchets display a rich variety of behaviors that vary markedly with the system parameters. Capturing the full range of these possibilities—and the transitions between them—as several parameters change is quite difficult with numerical solutions alone.

There are several categories of models for stochastic ratchets. The temporal variations of the external force can be a deterministic function (usually periodic [7,9,14]), or can be a stochastic process with nonzero correlation time [1,15]. Stochastic forcing is usually taken to be a stationary Markov stochastic process with a discrete or continuous state space [4–6,11,12,15–18]. Two possible forms for the spatial structure of the external force have received most attention: the "fluctuating force" and "fluctuating barrier" cases [4,12].

The first is the case where the force is constant in space; that is, the driving noise is additive [1,16,18]. An example of the second case is when the shape of the periodic potential changes randomly in time; this is an example where the driving noise is multiplicative [3,19,20].

There are two types of noise present in a ratchet driven by an external stochastic force. The first noise stems from thermal fluctuations, which in the Langevin and Smoluchowski framework are described by diffusion. In other words, the diffusion is the result of internal thermal interparticle interactions and follows the fluctuation-dissipation principle. It is well known that such diffusion alone cannot perform useful work in the steady state. The second noise—the external force—is usually taken to be a stochastic process with nonzero correlation time. For example, in biological systems these fluctuations may arise from intermittent chemical reactions which affect the distribution of electric charge and therefore alter the electric potential. These fluctuations can perform useful work, since they are driven by an external energy source (e.g., ATP molecules) [2,4,8,10].

In this paper, we consider a two-state stochastic fluctuating force model. In the liquid (high damping) phase, the diffusive dynamics of a particle in a thermal bath can be reduced from the Langevin second order equation to the Smoluchowski first order equation. We consider one-dimensional motion, where the particle position is denoted by x(t). Our nondimensionalized model for the particle dynamics is

$$\dot{x}(t) = -U'(x) + \sqrt{2D}\dot{w}(t) + \xi(t), \tag{1}$$

where U(x) is the deterministic potential, $\dot{w}(t)$ denotes standard Gaussian white noise, and $\xi(t)$ is a stochastic process independent of $\dot{w}(t)$ [$\xi(t)$ will be specified below].

There are three time scales that need to be considered in these problems. (The very short time interval between thermal scattering events has been removed by the Smoluchowski approximation.) The first time scale is characteristic of the force fluctuations, $\xi(t)$. We denote this time scale by τ . The second time scale, 1/D, is proportional to the time it

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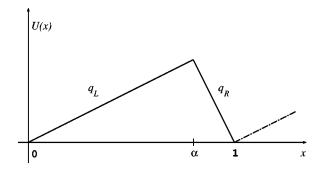


FIG. 1. Potential in a typical periodic sharp ratchet. Here $\alpha = -q_R/(q_L-q_R)$, with slopes denoted by q_L and q_R . (All variables are dimensionless in this and other figures.)

takes a particle to diffuse a unit distance. The third time scale is associated with the deterministic dynamics; this time is proportional to $\max[1/|U''(x)|^{1/2}]$. In any given model problem (1), the relationships among these three time scales are a key factor in determining the steady-state particle current.

A case when the force fluctuations occur more rapidly than the other two time scales has been studied by using asymptotic and numerical methods [11]. In this problem, the steady-state current is proportional to τ^3 as $\tau \to 0$. The asymptotic analysis breaks down when the dynamics time scale is significantly shorter than both τ and 1/D, since the coefficient of τ^3 diverges as $\max |U''(x)| \to \infty$. This happens when the force U'(x) changes abruptly over a very small distance. In such a case, we say that the potential has a sharp corner. We model this corner as perfectly sharp, so that U'(x) is only piecewise continuous. Numerical results indicate that with such a potential, the steady-state current is proportional to $\tau^{5/2}$ as $\tau \to 0$, instead of the τ^3 that occurs with smooth potentials [18].

We consider the simplest such potential over the entire real line, which is piecewise linear and periodic:

$$U(x) = \begin{cases} q_L(x-n) & x \in (n, \alpha+n) \\ q_R(x-n-1) & x \in (\alpha+n, n+1) \end{cases} n = 0, \pm 1, \pm 2, \dots,$$

where $\alpha \equiv -q_R/(q_L-q_R)$ (see Fig. 1). Without loss of generality we assume that $q_L > 0$, $q_R < 0$, and we have set the period of the potential to be 1. We take the fluctuating force $\xi(t)$ to be the zero mean symmetric telegraph process, taking on values $\pm a$ with exponentially distributed switching times, with parameter $1/(2\tau)$. In order to ensure the existence of a steady-state current, even in the absence of diffusion, we also assume that $a > \max\{q_L, |q_R|\}$, so that the force alternates between positive and negative.

The problem posed above can be solved in closed form, with the solution expressed in terms of the roots of a fourth order polynomial (see Sec. III). Indeed, this is one reason that this U(x) has been widely used in previous modeling efforts [1,4,12,18]. The exact solution is algebraically very complicated and gives no direct insight. We derive simpler and more useful asymptotic expressions for the steady-state current J for all four possible combinations of D small and large, τ small and large. (We keep the jump size a independent of D and τ in these limiting cases.) The order in which these limits are taken is important in some cases. The asymptotic dependence of J in all of these regimes is system-

atically and rigorously calculated. Some aspects of onedimensional dynamics driven by fast ($\tau \leq 1$) jump noise have been studied previously [21], in the case D=0. It was shown that the correct asymptotic expansion is in powers of $\tau^{1/2}$; however, in the case where U(x) is smooth, all of the coefficients of fractional powers of τ in the expansion of Jturn out to be zero. In the present model, it is necessary to retain the fractional powers of τ to get the correct current.

The derivation of our results is straightforward in principle, but very lengthy in practice; the procedure we developed is outlined in Sec. III. The results were checked using direct numerical solutions of the fourth order polynomial, followed by numerical solution of the linear system of equations for the steady-state probability $\mathbf{p}(x,\xi)$.

We find that $J = O(\tau^2 \exp[-(D\tau)^{-1/2}]) + O(\tau^{5/2})$ for small τ . For $D \le O(1)$ as $\tau \to 0$, the first term is exponentially small and the numerical prediction that $J = O(\tau^{5/2})$ is verified. However, for large $D \ge O(1/\tau)$ as $\tau \to 0$, the first term affects the magnitude of J. Keeping this term is essential to understand the dependence of J on D in the small τ case, as D changes from small to large. This result would be difficult to obtain from purely numerical solutions, and illustrates the additional insight that analytical asymptotic methods can bring to the solution of a problem. We also find that for small τ , there is a nonzero value of D that maximizes the current, and we derive an approximate equation for this optimal D (28). These results show that J can be asymptotically larger for sharp ratchets than for smooth ratchets, and also show the conditions that are needed to obtain the maximal current.

When $D \le 1$, we find that J is algebraic in D. The size of the current varies from transcendentally small to O(1) as τ changes from asymptotically small to large. The case when both $D \le 1$ and $\tau \le 1$ is where the order of the limiting operations matters: $D \le \tau \le 1$ is different than $\tau \le D \le 1$. The transition between these two regimes occurs when $D = O(\tau) \le 1$; the current is transcendentally small in this limit. When $D \ge 1$, the current vanishes algebraically as $1/D^4$ for arbitrary τ . These two limits are why there is a D that produces a maximal current for small enough τ . For larger τ , J is monotonically decreasing in D.

Biological systems have presumably evolved towards maximum efficiency, and technological systems should be designed to achieve maximum efficiency. Based on our results, we expect that the widely used sharp ratchet models will be found to be very applicable to scientific and engineering problems, not just for the fact that such models can be solved in closed form, but because they will also be excellent approximations to potentials found in the real world.

II. FORMULATION OF THE SOLUTION

The stochastic differential equation for the particle position x(t) is

$$\dot{x}(t) = -U'(x) + \sqrt{2D}\dot{w}(t) + \xi(t).$$
 (2)

The steady-state transition probability of the twodimensional process $(x(t), \xi(t))$, $\mathbf{p} = \mathbf{p}(x, \xi)$, satisfies the forward master equation

$$-\frac{\partial}{\partial x}[\mathbf{S}(x)\mathbf{p}] + D\frac{\partial^2 \mathbf{p}}{\partial x^2} + \frac{1}{\tau}\mathbf{W}\mathbf{p} = 0,$$
 (3)

where

$$\mathbf{S}(x) \equiv -U'(x)\mathbf{I} + \begin{bmatrix} a & 0 \\ 0 & -a \end{bmatrix} \equiv -U'(x)\mathbf{I} + \mathbf{\Xi},$$

and the forward transition state matrix of the process $\xi(t)$ is given by

$$\mathbf{W} = \begin{bmatrix} -1/2 & 1/2 \\ 1/2 & -1/2 \end{bmatrix}.$$

We calculate the steady-state probability current in the x variable. Denoting by $\mathbf{Y}^T = [1,1]$ the left eigenvector of \mathbf{W} , corresponding to the zero eigenvalue, we have

$$-\frac{\partial}{\partial x}J \equiv \frac{\partial}{\partial x}\mathbf{Y}^T \left[D\frac{\partial \mathbf{p}}{\partial x} - \mathbf{S}(x)\mathbf{p}\right] = 0.$$

Hence the current J is constant in x and is given by

$$J = -\mathbf{Y}^{T} \left[D \frac{\partial \mathbf{p}}{\partial x} - \mathbf{S}(x) \mathbf{p} \right] = \text{const.}$$
 (4)

We study the dependence of $J=J(D,\tau)$ on the diffusion coefficient D and the mean time between the jumps 2τ .

We solve exactly the master equation (3) in each of the constant force intervals $(0,\alpha)$ and $(\alpha,1)$. We determine constants of integration by requiring continuity, periodicity, and jump conditions. Denoting by $\mathbf{p}(x,q_L)$ the solution on $(0,\alpha)$, and by $\mathbf{p}(x,q_R)$ the solution on $(\alpha,1)$, we write these conditions as continuity at α ,

$$\mathbf{p}(x=\alpha,q_R) - \mathbf{p}(x=\alpha,q_L) = 0; \tag{5}$$

continuity and periodicity at x = 0,1,

$$\mathbf{p}(x=1,q_R) - \mathbf{p}(x=0,q_I) = 0;$$
 (6)

the jump in the derivative of \mathbf{p} at x=0 and x=1 with the periodicity of \mathbf{p} ,

$$D\!\left[\frac{\partial\mathbf{p}}{\partial x}(x=1,q_R) - \frac{\partial\mathbf{p}}{\partial x}(x=0,q_L)\right] + (q_R - q_L)\mathbf{p}(x=0,q_L) = 0;$$

$$(7)$$

the steady state of the telegraph noise,

$$\int_{0}^{\alpha} \mathbf{p}(x, q_L) dx + \int_{\alpha}^{1} \mathbf{p}(x, q_R) dx = \begin{bmatrix} 1/2 \\ 1/2 \end{bmatrix}. \tag{8}$$

[Conditions (5–8) imply the jump condition at $x = \alpha$,

(3)
$$D\left[\frac{\partial \mathbf{p}}{\partial x}(x=\alpha,q_R) - \frac{\partial \mathbf{p}}{\partial x}(x=\alpha,q_L)\right] + (q_R - q_L)\mathbf{p}(x=\alpha,q_L)$$
$$= 0,$$

so this condition need not be explicitly used.]

We denote by $\mathbf{X}_1 = [1,1]^T$ and $\mathbf{X}_2 = [1,-1]^T$ the right eigenvectors of \mathbf{W} , with the eigenvalues $\mu_1 = 0$ and $\mu_2 = -1$, respectively. We write the solution to the master equation (3) as

$$\mathbf{p}(x, q_{R(L)}) = C_1^{R(L)} \mathbf{X}_1 + \sum_{i=2}^4 C_i^{R(L)} \mathbf{p}_i^{R(L)}, \qquad (9)$$

where $\mathbf{p}_{i}^{R(L)}$ is given by \mathbf{p}_{i} in Eq. (10) with q replaced by $q_{R(L)}$,

$$\mathbf{p}_{i} = \left(\mathbf{X}_{1} + \frac{D\rho_{i} + q}{a}\mathbf{X}_{2}\right) \exp(\rho_{i}x), \tag{10}$$

and where $\{\rho_i, i=2,3,4\}$ is the set of nonzero roots of the algebraic equation

$$D^{2}\rho^{4} + 2Dq\rho^{3} + \left[q^{2} - a^{2} - \frac{1}{\tau}D\right]\rho^{2} - \frac{1}{\tau}q\rho = 0.$$
 (11)

We impose the conditions (5–8) to determine the eight constants $\{C_i^{R(L)}\}$. Using the fact that $\mathbf{Y}^T\mathbf{X}_2=0$, together with the form (9) of the solution in Eq. (4), we find that

$$J = -2q_R C_1^R = -2q_L C_1^L$$
.

We solve the system given by Eqs. (3), (5)-(8) in the asymptotic limits of $D \le 1$, $D \ge 1$, $\tau \le 1$, and $\tau \ge 1$. To this end, in a specified asymptotic limit, we solve Eq. (11) for the roots $\rho^{(i)}$ in the form of an asymptotic series (see the Appendix), write the solution (9), and then solve the system of eight equations for the constants $C_i^{R(L)}$. These constants, and hence the current, are functions of the parameters D and τ through exponential and pre-exponential terms. The preexponential terms are expanded in asymptotic power series; the exponential factors are kept in this form throughout the calculation, since they may be transcendentally large or small. The asymptotic interplay between these exponential and algebraic terms requires careful analysis. In particular, the validity of an asymptotic formula for the current depends on the validity of the asymptotic expansion of the roots of Eq. (11). Though the procedure of finding the solution may seem to be straightforward, its implementation (described in Sec. III below) is nontrivial.

This procedure can be generalized to calculate asymptotic expansions for the current in an arbitrary periodic nonsymmetric sharp potential. The first step is to find the asymptotic solution to the master equation (3) on each interval where the force is continuous. The form of this expansion depends on

the chosen asymptotic limit. For example, if $\tau \ll 1$ we seek \mathbf{p} in the WKB form $\mathbf{p} = \exp[-\psi/\sqrt{\tau}]\mathbf{k}$ [21]. For the case $D \ll 1$, \mathbf{p} also has a WKB form $\mathbf{p} = \exp[-\phi/D]\mathbf{k}$. Then constants of integration are determined by employing the periodicity, continuity, and marginal conditions analogous to Eqs. (5)–(8).

III. SOLUTION METHODS

We performed symbolic and numerical calculations using MAPLE V (Waterloo Software), running on a 400-MHz Pentium II Linux-based system. The symbolic asymptotic solutions were checked against direct numerical solutions, computed with up to 50 significant digits. Such precision was necessary when multiplying exponentially large and exponentially small terms. Symbolic calculations took from minutes to days, and had to be organized carefully for MAPLE V to be able to handle their complexity.

We solved the system [(5)-(8)] of eight equations with eight unknowns, representing the amplitudes of the four elementary solutions to Eq. (3) in each subinterval. After simple row operations the matrix of the system \mathbf{M} has the structure

$$\mathbf{M} = \begin{bmatrix} 1 & m_{12} & m_{13} & m_{14} & -1 & m_{16} & m_{17} & m_{18} \\ 0 & m_{22} & m_{23} & m_{24} & 0 & m_{26} & m_{27} & m_{28} \\ 0 & m_{32} & m_{33} & m_{34} & 0 & m_{36} & m_{37} & m_{38} \\ 0 & m_{42} & m_{43} & m_{44} & 0 & m_{46} & m_{47} & m_{48} \\ 0 & m_{52} & m_{53} & m_{54} & m_{55} & m_{56} & m_{57} & m_{58} \\ 0 & m_{62} & m_{63} & m_{64} & 0 & m_{66} & m_{67} & m_{68} \\ 0 & m_{72} & m_{73} & m_{74} & 1 & m_{76} & m_{77} & m_{78} \\ 0 & m_{82} & m_{83} & m_{84} & 0 & m_{86} & m_{87} & m_{88} \end{bmatrix}$$

and the right hand side is $\mathbf{b} = [0, \dots, 0, 1, 0]^T$. We solved the system $\mathbf{Mc} = \mathbf{b}$ using Cramer's rule, where \mathbf{c} is the vector of the $C_i^{R(L)}$ coefficients.

For illustration, we describe the symbolic calculation of $\det[\mathbf{M}]$. This determinant has 1440 terms, each being a product of six or seven of the m_{ij} ; this expansion is easily calculated with MAPLE V in terms of the generic m_{ij} . In each of the asymptotic limits considered (D small and large, τ small and large), we construct the asymptotic expansion of the entries m_{ij} in powers of the expansion parameter (τ or D). For each of 1440 terms we substitute these expansions of the expansion parameter. From each of the powers of the expansion parameter. From each term in the determinant sum, each coefficient in the expansion is fully multiplied out (often yielding an expression with dozens of terms). The coefficients of each power are appended to an output file; when calculating the expansion up to order k, we construct

k+1 files, so that the pth file contains the coefficient of the pth power of the expansion parameter. This coefficient is written so separate lines of the file contain its separate summands. After all 1440 terms in the determinant sum are processed in this way, the coefficient of the pth power of the expansion parameter can be obtained by adding up all the lines of the pth file. In some cases, these files contain over 2×10^6 lines, so it is impossible to carry this out directly within MAPLE V due to program limitations on the complexity of algebraic expressions, and also due to the amount of intermediate memory needed; this is the motivation for computing the expansion of one determinant term at a time and collecting its coefficients into files. (When adding up the coefficient files directly, at about 30 000 lines the system is overwhelmed and all available memory-in this case about 360 megabytes—is exhausted.) Many of the expressions in the files would cancel or combine if added directly (e.g., $3abc+\cdots+7abc+\cdots+2abc$, where there might be thousands of terms hidden by the ellipses). We developed a technique to add up such large expressions, under the assumption (or hope) that they will eventually collapse to a manageable set of terms. We sort each of the files by lines in the normal alphabetic order (outside MAPLE V, using the Unix sort utility). Then we read a file into MAPLE V and add all these ordered lines up, one at a time. The sorting tends to bring like subexpressions close together so that combination or cancellation can occur before the sum becomes too bulky for MAPLE V to handle. There is sufficient cancellation with this method so that the system memory does not become exhausted. Adding up 2×10^6 lines in this fashion takes about 24 CPU hours. As will be seen below, in most cases the final expressions are vastly simpler than the intermediate results.

IV. NO DIFFUSION ($D \equiv 0$) AND SMALL DIFFUSION ($D \ll 1$)

In this section first we calculate the current in the case of no diffusion, D=0, and then study how small diffusion, $D \ll 1$, affects the current. In the case D=0, we first solve the master equation (3) to find

$$\mathbf{p}(x, q_{R(L)}) = C_1^{R(L)} \mathbf{X}_1 + C_2^{R(L)} \left(\frac{a}{q_{R(L)}} \mathbf{X}_1 + \mathbf{X}_2 \right) \exp(\lambda_{R(L)} x),$$

where $\lambda_{R(L)} = q_{R(L)}/[(q_{R(L)}^2 - a^2)\tau]$. We calculate constants of integration by requiring the jump condition at $x = \alpha$, $\mathbf{S}(\alpha^+)\mathbf{p}(\alpha^+,q_R) - \mathbf{S}(\alpha^-)\mathbf{p}(\alpha^-,q_L) = 0$, and the stationary marginal transition probability of the noise, as in Eq. (8). (This jump condition together with Eq. (8) and the periodicity of \mathbf{p} [i.e., $\mathbf{p}(x=1^+,q_L) = \mathbf{p}(x=0^+,q_L)$, $\mathbf{p}(x=0^-,q_R) = \mathbf{p}(x=1^-,q_R)$] implies the jump condition at x=0/1 is $\mathbf{S}(1^-)\mathbf{p}(1^-,q_R) - \mathbf{S}(0^+)\mathbf{p}(0^+,q_L) = 0$.) Then we calculate the current, $J(D=0,\tau) \equiv J_{Dzero}(\tau) = -\mathbf{Y}^T\mathbf{S}(x)\mathbf{p}$, to find

$$J_{Dzero}(\tau) = \frac{-q_R^2 q_L^2 [\exp(\lambda_R \alpha) - \exp(\lambda_R + \lambda_L \alpha)]}{(q_R + q_L) [\exp(\lambda_R \alpha) - \exp(\lambda_R + \lambda_L \alpha)] + \tau a^2 (q_R - q_L)^2 [\exp(\lambda_L \alpha) - 1] [\exp(\lambda_R \alpha) - \exp(\lambda_R)]}.$$
 (12)

We note that when $q_R \rightarrow -q_L$ (the symmetric potential), $J_{Dzero}(\tau) \rightarrow 0$. In the asymptotic limit of slow jumps whose size is O(1), (i.e., when $\tau \rightarrow \infty$) we have

$$J_{Dzero}(\tau) = \frac{q_L q_R (q_L + q_R)}{a^2 - (q_L + q_R)^2} + O\left(\frac{1}{\tau}\right) \equiv J_{Dzero}(\infty) + O\left(\frac{1}{\tau}\right). \tag{13}$$

In the asymptotic limit of fast jumps of O(1), (i.e., when $\tau \rightarrow 0$), we find that J_{Dzero} is exponentially small in τ :

$$J_{Dzero}(\tau) = \frac{1}{\tau} \frac{q_R^2 q_L^2}{a^2 (q_R - q_L)^2} e^{\lambda_L \alpha} [1 + O(e^{\lambda_R (\alpha - 1)})]$$
(14)

$$\equiv J_{Dzero}(0)[1 + O(e^{\lambda_R(\alpha - 1)})]. \tag{15}$$

As τ increases, the current increases from exponentially small values in $1/\tau$ to a value algebraically close to a constant.

In the diffusion limit of $\xi(t)$ (i.e., fast large jumps with $\tau = \epsilon^2 \tilde{\tau}$, $a = \tilde{a}/\epsilon$, and $\epsilon \to 0$), we have

$$\begin{split} J_{Dzero}(\tau) &= \epsilon^2 \frac{(q_L + q_R)q_L^3 q_R^3 \exp(-q_R \alpha/\mathcal{D})}{\widetilde{a}^6 \widetilde{\tau}^2 (q_L - q_R)^2 [\exp(-q_R \alpha/\mathcal{D}) - \exp(-q_R/\mathcal{D})] [\exp(-q_L \alpha/\mathcal{D}) - 1]} + O(\epsilon^3) \\ &\equiv J_{Dzero}^{diff} + O(\epsilon^3), \end{split}$$

where $\mathcal{D} = \tilde{\tau} \tilde{a}^2$ is the effective diffusion coefficient.

We next consider the case of $D \le 1$. Nonzero diffusion has singular smoothing effects on the system. While the marginal transition probability function in x of Eq. (2) with $D \equiv 0$ suffers discontinuities at the points where the force is discontinuous, the marginal transition probability in the case of $D \ne 0$ is smooth; see Fig. 2.

Effects of small D on the current are singular in a different manner. We find the current

$$J_{smallD}(D,\tau) = J_{Dzero}(\tau) + DJ_{smallD}^{(1)}(D,\tau) + O(D^2), \tag{16} \label{eq:16}$$

where J_{Dzero} is exactly the zero-diffusion current in (12). We find

$$J_{smallD}^{(1)}(D,\tau) = J_{smallD}^{(1)}(0,\tau) + O(e^{-a/D}).$$
 (17)

Figure 3 shows the graph of the analytical formula for

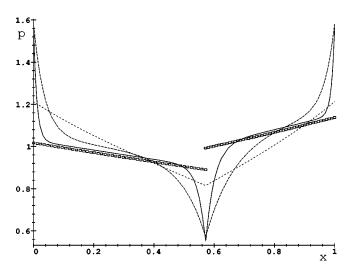


FIG. 2. Marginal transition probability for q_L =3/4, q_R =-1, a=2, when τ =1 and various D. Short dashes, D=1; dashes, D=0.1; solid line, D=0.03; boxes, D=0.

 $J_{smallD}^{(1)}(0,\tau)$. The exact formula for $J_{smallD}^{(1)}(0,\tau)$ is extremely lengthy (many pages), so we show its graph and study its asymptotic properties in τ . For $\tau \gg 1$ [$\xi(t)$ is a slowly changing telegraph process], we find

$$J_{smallD}^{(1)}(0,\tau) = 2 \frac{(-q_L + q_R)^2 (q_R + q_L) a}{(q_L + q_R + a)^2 (q_L + q_R - a)^2} + O\left(\frac{1}{\tau}\right)$$

$$\equiv J_{smallD}^{(1)}(0,\infty) + O\left(\frac{1}{\tau}\right)$$
(18)

while, for $\tau \leq 1$,

$$J_{smallD}^{(1)}(0,\tau) = \left[\frac{1}{\tau^3} \frac{(q_L^2 + a^2)q_L^3 q_R^3}{a^2 (q_R - q_L)^3 (-q_L + a)^3 (a + q_L)^3} + O\left(\frac{1}{\tau^2}\right)\right] e^{q_L \alpha / [(q_L^2 - a^2)\tau]} (1 + \text{TST}), \quad (19)$$

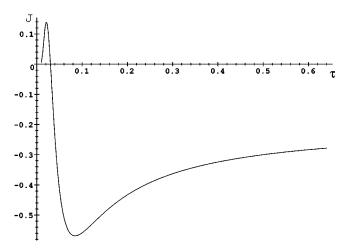


FIG. 3. Graph of $J_{smallD}^{(1)}(0,\tau)$ vs τ for $q_L=3/4, q_R=-1, a=2$.

where TST denotes a transcendentally small term. Here we have

$$TST = O(\max[e^{-q_R q_L/[(q_L - q_R)(q_R^2 - a^2)\tau]}, e^{2q_L \alpha/[(q_L^2 - a^2)\tau]}]).$$

[In the derivation of Eq. (19) we explicitly assume that $q_L \neq -q_R$ when we disregard exponentially small terms. This is why Eq. (19) does not reduce to zero when $q_L + q_R = 0$, although the exact formula for $J_{smallD}^{(1)}(0,\tau)$ does simplify to zero in this case.]

For a fixed $\tau \ll 1$, the current $J_{smallD}(D, \tau)$ (as a function of D) approaches a transcendentally small value with a transcendentally small slope as $D \rightarrow 0$. We note that $J_{Dsmall}^{(1)}(0,\tau)$ takes on positive values for $\tau \ll 1$, according to Eq. (19), while it takes on negative values for $\tau \gg 1$, according to Eq. (18). Hence there are values τ^* and τ^{**} such that $J_{Dsmall}^{(1)}(0, au) > 0$ for $au < au^*$, and $J_{Dsmall}^{(1)}(0, au) < 0$ for au $>\tau^{**}$. Numerical evaluation of the exact formula for $J_{smallD}^{(1)}(0,\tau)$ suggests that $\tau^{*}=\tau^{**}$; compare Fig. 3. In the discussion below we assume that this holds [i.e., $J_{Dsmall}^{(1)}(0,\tau)$ has only one zero for $\tau \in (0,\infty)$]. In Sec. VI we show that as $D \rightarrow \infty, J(D, \tau) \rightarrow 0$. For a fixed value of τ $<\tau^*$, the slope of $J(D,\tau)$ is positive for $D \le 1$, and J is an increasing function of D, while for $D \gg 1$, J is a decreasing function of D. Hence J achieves a maximum as a function of D, if $\tau < \tau^*$. We conclude that for each $\tau < \tau^*$, there is a value of D which maximizes the current. For $\tau > \tau^*$, the current J is a decreasing function of D. Hence for τ sufficiently small, a little bit of diffusion increases the current, but a lot of diffusion diminishes it.

The analysis of this section is valid for values of τ such that $\tau \gg D$. To see this, we note that the terms in the asymptotic formulas for the roots in Eq. (A1) depend on the quotient D^{m-1}/τ^m . We explicitly assume that $D \ll 1$ and higher order (disregarded) terms are asymptotically smaller than those kept, which implies $\tau \gg D$. The range of validity of the asymptotic expansion is important to keep in mind when taking the iterated limit of $D \ll 1$ and $\tau \ll 1$. The result (16) is valid for $D \ll 1$ and $\tau \gg D$. The validity of the result breaks down when $\tau = O(D)$ or smaller.

Since $J_{smallD}^{(1)}$ can be negative, one might be tempted to postulate current reversal; by adding just enough of $J_{smallD}^{(1)}$ in Eq. (16) to J_{Dzero} in Eq. (12)—that is, by selecting the just right value of the diffusion coefficient D—one might be able to change the sign of the current as a function of τ . However, this only happen for values of $\tau \ll D$, when the above asymptotics are not valid. We do not observe current reversal in our ratchet model.

V. FAST JUMP NOISE, $\tau \ll 1$

In the case of $\tau \leq 1$ we find that the current J is given by

$$J_{small\tau}(D,\tau) = \tau^2 J_4 + \tau^{5/2} J_5 + O(\tau^3). \tag{20}$$

The coefficients J_4 and J_5 are given by

$$J_{4} = \frac{1}{2} \frac{1}{D^{3}} q_{L}^{2} q_{R}^{2} a^{2} \frac{\left(-e^{1/(\sqrt{D}\sqrt{\tau})} + e^{2\alpha/(\sqrt{D}\sqrt{\tau})}\right) e^{-q_{L}\alpha/(2D)}}{\left(e^{-q_{L}\alpha/D} - 1\right) e^{\alpha/(\sqrt{D}\sqrt{\tau})} \left(e^{1/(\sqrt{D}\sqrt{\tau})} - 1\right)},\tag{21}$$

$$\begin{split} J_5 = & \frac{1}{4} \frac{1}{D^{7/2}} a^2 q_L^2 q_R^2 \mathcal{F}(-q_L e^{4\alpha/(\sqrt{D}\sqrt{\tau})} \mathcal{F} - q_L e^{2(1+\alpha)/(\sqrt{D}\sqrt{\tau})} \mathcal{F} + q_L e^{2\alpha/(\sqrt{D}\sqrt{\tau})} \mathcal{F} + q_L e^{2/(\sqrt{D}\sqrt{\tau})} \mathcal{F} - q_L e^{(1+\alpha)/(\sqrt{D}\sqrt{\tau})} + q_L e^{(1+3\alpha)/(\sqrt{D}\sqrt{\tau})} \mathcal{F} + q_L e^{2\alpha/(\sqrt{D}\sqrt{\tau})} \mathcal{F} + q_L e^{2/(\sqrt{D}\sqrt{\tau})} \mathcal{F} - q_L e^{(1+\alpha)/(\sqrt{D}\sqrt{\tau})} + q_L e^{(1+3\alpha)/(\sqrt{D}\sqrt{\tau})} \mathcal{F} \\ & + q_L e^{(1+3\alpha)/(\sqrt{D}\sqrt{\tau})} e^{q_L \alpha/D} - q_L e^{(1+\alpha)/(\sqrt{D}\sqrt{\tau})} e^{q_L \alpha/D} - q_R e^{2/(\sqrt{D}\sqrt{\tau})} \mathcal{F} + q_R e^{(2+\alpha)/(\sqrt{D}\sqrt{\tau})} - q_R e^{3\alpha/(\sqrt{D}\sqrt{\tau})} + q_R e^{2\alpha/(\sqrt{D}\sqrt{\tau})} \mathcal{F} \\ & - q_R e^{2(1+\alpha)/(\sqrt{D}\sqrt{\tau})} \mathcal{F} + q_R e^{(2+\alpha)/(\sqrt{D}\sqrt{\tau})} e^{q_L \alpha/D} + q_R e^{4\alpha/(\sqrt{D}\sqrt{\tau})} \mathcal{F} - q_R e^{3\alpha/(\sqrt{D}\sqrt{\tau})} e^{q_L \alpha/D}) / [e^{2\alpha/(\sqrt{D}\sqrt{\tau})} \mathcal{F} + q_R e^{2\alpha/(\sqrt{D}\sqrt{\tau})} \mathcal{F} - q_R e^{3\alpha/(\sqrt{D}\sqrt{\tau})} e^{q_L \alpha/D}] \\ & \times (e^{1/(\sqrt{D}\sqrt{\tau})} - 1)^2 (-1 + e^{q_L \alpha/D})^2] \end{split}$$

where $\mathcal{F} = e^{q_L \alpha/(2D)}$.

In general, the coefficient J_4 is exponentially small in $\sqrt{\tau}$. Specifically, if $-q_R > q_L$ then we have

$$J_4 = j_4 e^{(\alpha - 1)/(\sqrt{D\tau})} [1 + O(e^{(1 - 2\alpha)/(\sqrt{D\tau})})],$$

where

$$j_4 = \frac{1}{2} \frac{1}{D^3} q_L^2 q_R^2 a^2 \frac{e^{q_L q_R / [2D(q_L - q_R)]}}{(e^{q_L q_R / [D(q_L - q_R)]} - 1)}.$$
 (22)

The nonexponentially small contribution to J comes from the coefficient j_5 defined below. Rearranging the terms in J_5 we find

$$J_5 = j_5 + j_5^L e^{-\alpha/(\sqrt{D\tau})} + j_5^R e^{-(1-\alpha)/(\sqrt{D\tau})} + \text{TST},$$

where

$$j_{5} = -\frac{1}{4} \frac{1}{D^{7/2}} (q_{L} + q_{R}) q_{R}^{2} q_{L}^{2} a^{2} \frac{e^{q_{L}\alpha/D}}{(-1 + e^{q_{L}\alpha/D})^{2}}, \quad (23)$$

$$j_{5}^{L} = \frac{1}{4} \frac{1}{D^{7/2}} a^{2} q_{R}^{3} q_{L}^{2} \frac{e^{q_{L}\alpha/(2D)} (1 + e^{q_{L}\alpha/D})}{(-1 + e^{q_{L}\alpha/D})^{2}},$$

$$j_{5}^{R} = \frac{1}{4} \frac{1}{D^{7/2}} a^{2} q_{R}^{2} q_{L}^{2} \frac{e^{q_{L}\alpha/(2D)} (1 + e^{q_{L}\alpha/D})}{(-1 + e^{q_{L}\alpha/D})^{2}}.$$

Hence with a transcendentally small error we have

$$J_{small}(D,\tau) = j_5 \tau^{5/2} + O(\tau^3). \tag{24}$$

We note that the analysis of this section is valid for $\tau \le 1$ and values of D which satisfy the conditions $D\tau \le 1$ and $D \ge \tau$. The first of these conditions results from the asymptotic arrangement of terms when solving the system of linear equations (5)–(8). The second condition stems from the assumption that higher order terms in the expansion of the roots in Eq. (A2) are asymptotically smaller than the lower order terms which are kept in the calculations.

Up to this point, in this section we have assumed that D = O(1). If we assume that $D \le 1$ (while $D \ge \tau$), then J_4 in Eq. (21) is exponentially small, both in τ and D. Specifically, we have

$$\begin{split} J_4 &= -\frac{1}{2} \frac{1}{D^3} q_L^2 q_R^2 a^2 e^{-q_L q_R/[2(q_L - q_R)D]} e^{-q_L/[(q_L - q_R)\sqrt{D\tau}]} \\ &\times [1 + O(e^{q_L q_R/[D(q_L - q_R)]})], \end{split}$$

and J_5 , or equivalently j_5 , becomes exponentially small in D. Hence in the iterated asymptotic limit $\tau \ll 1, D \ll 1$ the current is exponentially small in D, and

$$J_{small\tau}(D,\tau) = -\frac{\tau^{5/2}}{D^{7/2}} (q_L + q_R) q_R^2 q_L^2 a^2 \exp(-q_L \alpha/D) + O(\tau^3) = O\left(\frac{\tau^{5/2}}{D^{7/2}} e^{-q_L \alpha/D}\right).$$
 (25)

We emphasize that the iterated limits $\tau \ll 1$, $D \ll 1$ and $D \ll 1$, $\tau \ll 1$ are not interchangeable; compare the result Eqs. (16) with (15) and (19).

If $D \gg 1$ then

$$j_5 = -\frac{1}{4} \frac{1}{D^{3/2}} a^2 (q_L + q_R) (q_L - q_R)^2 + O\left(\frac{1}{D^{7/2}}\right), \quad (26)$$

so that we have

$$\begin{split} J_{small\,\tau}(D,\tau) &= -\frac{\tau^{5/2}}{4D^{3/2}}a^2(q_L + q_R)(q_L - q_R)^2 \\ &+ O\!\left(\frac{\tau^{5/2}}{D^{7/2}},\tau^3\right) \\ &= O\!\left(\frac{\tau^{5/2}}{D^{3/2}}\right). \end{split} \tag{27}$$

We observe that for a fixed $\tau \ll 1$, the dependence of the current, $J_{small\tau}(D,\tau)$, on D changes from exponential to algebraic as D varies from values asymptotically small to asymptotically large. As D increases, the current increases first through exponentially small values, it achieves its maximum, and finally decays algebraically to zero. According to Eq. (23) the maximum value of the current is achieved for the value of D which is the solution to the transcendental equation

$$2q_Lq_R(1+e^{q_L\alpha/D})-7D(q_L-q_R)(1-e^{q_L\alpha/D})=0. \hspace{0.5cm} (28)$$

This equation predicts the current-maximizing D with a precision determined by the asymptotic calculations.

VI. SLOW JUMP NOISE $(\tau \gg 1)$

We solve Eq. (11) in the asymptotic limit of $\tau \gg 1$, while keeping D fixed. For the asymptotic formulas, for the roots in Eq. (A3) to be valid we must have also $\tau \gg D$. We calculate the current to obtain

$$J_{large\tau}(D,\tau) = J_{large\tau}^{(0)}(D) + O\left(\frac{1}{\tau}\right). \tag{29}$$

The exact formula for the leading order term $J^{(0)}_{large\tau}(D)$ is lengthy (about one page), and by itself does not give any insight. To get more information we study it in asymptotic limits.

If $D \gg 1$ then we have

$$J_{large\tau}^{(0)}(D) = \frac{1}{D^4} \frac{1}{360} \frac{a^2 q_L^3 q_R^3 (q_L + q_R)}{(q_L - q_R)^4} + O\left(\frac{1}{D^5}\right), (30)$$

so that the current decays to zero algebraically at a rate independent of τ .

If $D \le 1$ then we have

$$J_{large\tau}(D) = \left[J_{Dzero}(\infty) + DJ_{smallD}^{(1)}(0,\infty) + O\left(D^{2}, \frac{1}{\tau}\right) \right] \times \left[1 + O(e^{-a/D}, e^{q_{R}(a - q_{L})/[D(q_{L} - q_{R})]}, e^{-q_{L}(q_{R} + a)/[D(q_{L} - q_{R})]} \right], \tag{31}$$

where $J_{Dzero}(\infty)$ and $J_{smallD}^{(1)}(0,\infty)$ are given by Eqs. (13) and (18), respectively. Hence the iterated limits of $\tau \gg 1$ and $D \ll 1$, and $D \ll 1$ and $\tau \gg 1$ give the same results; they are interchangeable.

In the asymptotic limit of $\tau \gg 1$ the telegraph noise changes slowly, staying in each of its values $\pm a$ on average for times of length 2τ . As $\tau \to \infty$ one of the levels of the noise a or -a is selected with probability 1/2, and the current J is the average (with respect to the stationary noise distribution) of the two currents obtained from the dynamics (2) with $\xi = a$ or $\xi = -a$. So, to leading order, $J_{large\tau}(D, \tau)$ is independent of τ , as shown in Eq. (29).

VII. STRONG DIFFUSION $(D \gg 1)$

Asymptotic expansion of the roots of Eq. (11) in the case of $D \gg 1$ is valid for $\tau \gg 1/D$; compare Eq. (A4). In this case, the exponential terms which depend on 1/D can be expanded in power series, so that the entries of the matrix (5)–(8) can be represented by asymptotic series in powers of 1/D. We calculate the current as

$$J_{largeD}(D,\tau) = \frac{1}{D^4} \frac{1}{360} \frac{a^2 q_L^3 q_R^3 (q_L + q_R)}{(q_L - q_R)^4} + O\left(\frac{1}{D^{9/2}}\right). \tag{32}$$

We note that to leading order the large D result is exactly the same as the result of the iterated limit $\tau \gg 1$ and $D \gg 1$; compare Eq. (30). The asymptotic limits of $D \gg 1$ and $\tau \gg 1$ are interchangeable. If the jumps are not too frequent ($\tau \gg 1/D$) then the strong diffusion smoothes and smears their effects, so that the current vanishes algebraically in D at a

rate independent of τ . This is in contrast to the case $\tau \leq 1$ and $D \geq 1/\tau$, when the current decays algebraically to zero in $D^{-3/2}$ at a rate proportional to $\tau^{5/2}$; compare Eqs. (26) and (27). If we take $\tau = D$ in Eqs. (26) and (27) then $J_{small\tau} = O(1/D^4)$, but the numerical factors in Eqs. (32) and (27) are different. Higher order terms in powers of τ in the series for Eq. (27) are needed to account for all terms of $O(1/D^4)$ when $\tau = 1/D$.

If $\tau \ll 1/D$ then the current is asymptotically smaller than $O(1/D^4)$, according to Eq. (27), and it decays algebraically in τ and D.

VIII. DISTINGUISHED LIMITS

The results of Secs. IV and V show that the iterated limits $D \ll 1$ and $\tau \gg 1$ are interchangeable. In contrast, the results of Secs. IV and VI show that the limits $\tau \ll 1$ and $D \gg 1$ are not interchangeable. We now show that Eq. (20) is valid uniformly for $D \gg \tau$, including $D = O(1/\tau)$ and $D \gg 1/\tau$. In particular, we show how Eq. (32) carries through the distinguished limit of $\tau = 1/D$ to the regime $\tau \ll 1$ in which Eq. (27) holds. To establish this result we substitute $D = 1/(k^2\tau)$ in Eq. (20) and then expand in a Taylor series in powers of τ to obtain, to leading order,

$$\begin{split} J_{small\tau}\!\!\left(\frac{1}{k^2\tau},\tau\right) &= -\frac{1}{4}(q_L\!-\!q_R)k^3a^2\tau^4\!\left(-\frac{q_R^2(-2E_L^2E_R\!-\!E_R^2\!+\!e^{2k}E_R^2\!-\!1\!+\!2E_R\!+\!E_L^2E_R^2)}{E_R^2}\right. \\ &\left.-\frac{q_L^2(-1\!-\!2E_LE_R^2\!-\!e^{2k}E_R^2\!+\!2E_L\!+\!E_R^2\!+\!E_L^2E_R^2)}{E_R^2}\right. \\ &\left.+2\frac{q_Lq_R(-1\!+\!E_LE_R)(E_LE_R\!-\!E_L\!+\!k\,E_L\!-\!k\,E_R\!-\!E_R\!+\!1)}{E_R^2}\right)\bigg/\left(e^k\!-\!1\right)^2, \end{split} \tag{33}$$

where

$$E_L = \exp\left(\frac{kq_L}{q_L - q_R}\right)$$
 and $E_R = \exp\left(\frac{kq_R}{q_L - q_R}\right)$.

If k=1 then Eq. (33) is the distinguished limit result of $\tau \ll 1$ and $D=1/\tau$. To obtain the expression for the current for the values of D even larger than $O(1/\tau)$ we now take the limit as $k \rightarrow 0$ in Eq. (33) to obtain

$$J_{small\tau,largeD} = \frac{1}{360} k^8 \tau^4 \frac{q_L^3 q_R^3 a^2 (q_R + q_L)}{(q_L - q_R)^4}.$$
 (34)

Recalling that $D = 1/(k^2 \tau)$, formulas (32) and (34) are identical.

The limits $\tau \ll 1$ and $D \ll 1$ are also not interchangeable. The transition between the results (19) (iterated limit $D \ll 1, \tau \ll 1$) and (25) (iterated limit $\tau \ll 1, D \ll 1$) occurs when $D = k \tau$, where k = O(1). The current is exponentially small, $J \sim \exp(-\kappa/D)$, with κ being proportional to the smallest (positive) root of the cubic equation

$$kY^3 + 2qY^2 + (q^2 - a^2 - k)Y - q = 0.$$

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APPENDIX: ASYMPTOTICS OF EIGENVALUES

We denote by $\rho^{(0)} = 0$ the zero eigenvalue of Eq. (11), and seek the expansions of the other roots of Eq. (11) in the various asymptotic limits. In the case $0 < D \le 1$, we obtain

$$\rho^{(2)} = \frac{q}{\tau(q^2 - a^2)} - \frac{D}{\tau^2} \frac{q(q^2 + a^2)}{(q^2 - a^2)^3} + O\left(\frac{D^2}{\tau^3}\right),$$

$$\rho^{(3)} = \frac{-q+a}{D} + \frac{1}{2} \frac{1}{\tau(-q+a)} - \frac{1}{8} \frac{D}{\tau^2} \frac{a+q}{(-q+a)^3 a} + O\left(\frac{D^2}{\tau^3}\right),\tag{A1}$$

$$\rho^{(4)} = -\frac{q+a}{D} - \frac{1}{2} \frac{1}{\tau(q+a)} + \frac{1}{8} \frac{D}{\tau^2} \frac{-q+a}{(a+q)^2 a} + O\left(\frac{D^2}{\tau^3}\right).$$

This expansion is valid for $\tau \gg D$.

In the asymptotic limit of $\tau \leq 1$, the asymptotic expansions of the eigenvalues are

$$\rho^{(2)} = -q/D + \tau \frac{a^2q}{D^2} - \tau^2 \frac{a^4q}{D^3} + O(\tau^3/D^4),$$

$$\rho^{(3)} = \frac{1}{\sqrt{D\tau}} - \frac{1}{2} \frac{q}{D} + \frac{1}{8} \frac{q^2 + 4a^2}{D^{3/2}} \sqrt{\tau} + O(\tau/D^2), \quad (A2)$$

$$\rho^{(4)} = -\frac{1}{\sqrt{D\tau}} - \frac{1}{2} \frac{q}{D} - \frac{1}{8} \frac{q^2 + 4a^2}{D^{3/2}} \sqrt{\tau} + O(\tau/D^2).$$

This expansion is valid for $D \gg \tau$.

In the asymptotic limit of $\tau \gg 1$, the asymptotic expansions of the eigenvalues are

(A4)

$$\rho^{(2)} = \frac{1}{\tau} \frac{q}{q^2 - a^2} - \frac{D}{\tau^2} \frac{q(a^2 + q^2)}{(q^2 - a^2)^3} + O\left(\frac{D^2}{\tau^3}\right), \qquad \rho^{(2)} = -\frac{q}{D} + \frac{1}{D^2} \frac{a^2 q}{\tau} + O\left(\frac{1}{D^3 \tau^2}\right),$$

$$\rho^{(3)} = \frac{-q + a}{D} - \frac{1}{2} \frac{1}{\tau} \frac{1}{q - a} + \frac{1}{8} \frac{D}{\tau^2} \frac{q + a}{(q - a)^3 a} + O\left(\frac{D^2}{\tau^3}\right), \qquad \rho^{(3)} = \frac{1}{\sqrt{D}\sqrt{\tau}} - \frac{1}{2} \frac{q}{D} + O\left(\frac{1}{D^{3/2}\sqrt{\tau}}\right),$$

$$\rho^{(4)} = -\frac{q + a}{D} - \frac{1}{2} \frac{1}{\tau} \frac{1}{q + a} - \frac{1}{8} \frac{D}{\tau^2} \frac{q - a}{(q + a)^3 a} + O\left(\frac{D^2}{\tau^3}\right). \qquad \rho^{(4)} = -\frac{1}{\sqrt{D}\sqrt{\tau}} - \frac{1}{2} \frac{q}{D} + O\left(\frac{1}{D^{3/2}\sqrt{\tau}}\right).$$

This expansion is valid for $\tau \gg D$.

The asymptotic expansion of the eigenvalues in the case of $D \gg 1$ is valid for $\tau \gg 1/D$, and is given by

In the actual calculations (cf. Sec. III), these expansions are needed to higher order, so that the m_{ij} are calculated with sufficient accuracy.

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